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PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	AUG 09	INSPEC enhanced with 1898-1968 archive
NEWS	4	AUG 28	ADISCTI Reloaded and Enhanced
NEWS	5	AUG 30	CA(SM)/CAplus(SM) Austrian patent law changes
NEWS	6	SEP 11	CA/CAplus enhanced with more pre-1907 records
NEWS	7	SEP 21	CA/CAplus fields enhanced with simultaneous left and right truncation
NEWS	8	SEP 25	CA(SM)/CAplus(SM) display of CA Lexicon enhanced
NEWS	9	SEP 25	CAS REGISTRY(SM) no longer includes Concord 3D coordinates
NEWS	10	SEP 25	CAS REGISTRY(SM) updated with amino acid codes for pyrrolysine
NEWS	11	SEP 28	CEABA-VTB classification code fields reloaded with new classification scheme
NEWS	12	OCT 19	LOGOFF HOLD duration extended to 120 minutes
NEWS	13	OCT 19	E-mail format enhanced
NEWS	14	OCT 23	Option to turn off MARPAT highlighting enhancements available
NEWS	15	OCT 23	CAS Registry Number crossover limit increased to 300,000 in multiple databases
NEWS	16	OCT 23	The Derwent World Patents Index suite of databases on STN has been enhanced and reloaded
NEWS	17	OCT 30	CHEMLIST enhanced with new search and display field
NEWS	18	NOV 03	JAPIO enhanced with IPC 8 features and functionality

NEWS EXPRESS JUNE 30 CURRENT WINDOWS VERSION IS V8.01b, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 26 JUNE 2006.

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8
NEWS X25	X.25 communication option no longer available

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 16:09:04 ON 05 NOV 2006

=>
Uploading
THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE
Do you want to switch to the Registry File?
Choice (Y/n):
Switching to the Registry File...
Some commands only work in certain files. For example, the EXPAND command can only be used to look at the index in a file which has an index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands which can be used in this file.

=> FILE REGISTRY

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 16:09:33 ON 05 NOV 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 3 NOV 2006 HIGHEST RN 912441-38-4
DICTIONARY FILE UPDATES: 3 NOV 2006 HIGHEST RN 912441-38-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

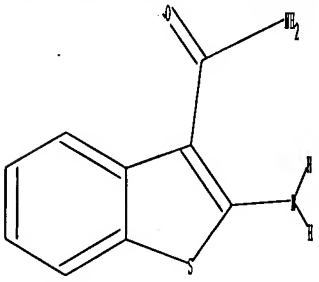
TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

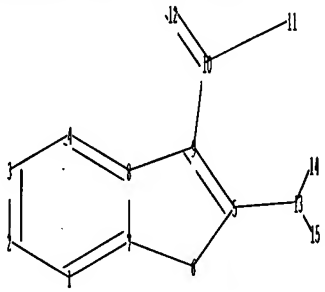
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10517111.str





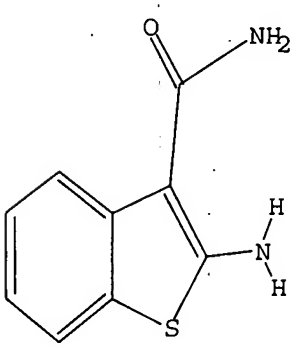
chain nodes :

10 11 12 13 14 15
ring nodes :
1 2 3 4 5 6 7 8 9
chain bonds :
5-13 9-10 10-11 10-12 13-14 13-15
ring bonds :
1-2 1-7 2-3 3-4 4-8 5-6 5-9 6-7 7-8 8-9
exact/norm bonds :
5-13 10-11 10-12
exact bonds :
5-6 5-9 6-7 8-9 9-10 13-14 13-15
normalized bonds :
1-2 1-7 2-3 3-4 4-8 7-8
isolated ring systems :
containing 1 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 16:09:46 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 36 TO ITERATE

100.0% PROCESSED 36 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 360 TO 1080
PROJECTED ANSWERS: 1 TO 80

L2 1 SEA SSS SAM L1

=> s l1 sss full
FULL SEARCH INITIATED 16:09:52 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 713 TO ITERATE

100.0% PROCESSED 713 ITERATIONS 4 ANSWERS
SEARCH TIME: 00.00.01

L3 4 SEA SSS FUL L1

=> FIL HCAPLUS
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	166.94	167.15

FILE 'HCAPLUS' ENTERED AT 16:09:57 ON 05 NOV 2006
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FILE COVERS 1907 - 5 Nov 2006 VOL 145 ISS 20
FILE LAST UPDATED: 3 Nov 2006 (20061103/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3
L4 2 L3

=> d l4 ibib abs hitstr tot

L4 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:238994 HCAPLUS
DOCUMENT NUMBER: 142:316820
TITLE: Preparation of hetero-bicyclic fused thieno-pyran compounds as antibacterial, antiviral, antitumor, and pharmaceutically active agents
INVENTOR(S): Koul, Anil; Klebl, Bert; Mueller, Gerhard; Missio, Andrea; Schwab, Wilfried; Hafenbradl, Doris; Neumann, Lars; Sommer, Marc-Nicola; Mueller, Stefan; Hoppe, Edmund; Freisleben, Achim; Backes, Alexander; Hartung, Christian; Felber, Beatrice; Zech, Birgit; Engkvist, Ola; Keri, Gyoergy; Oerfi, Laszlo; Banhegyi, Peter; Greff, Zoltan; Horvath, Zoltan; Varga, Zoltan; Marko, Peter; Pato, Janos; Szabadkai, Istvan; Szekelyhidi,

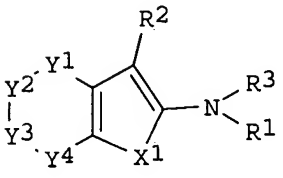
Zsolt; Waczek, Frigyes
PATENT ASSIGNEE(S): Axxima Pharmaceuticals A.-G., Germany
SOURCE: PCT Int. Appl., 259 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005023818	A2	20050317	WO 2004-EP10161	20040910
WO 2005023818	A3	20050825		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004270394	A1	20050317	AU 2004-270394	20040910
EP 1670804	A2	20060621	EP 2004-786934	20040910
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				

PRIORITY APPLN. INFO.:

EP 2003-20616	A	20030910
US 2003-502606P	P	20030915
EP 2004-4891	A	20040302
US 2004-551341P	P	20040310
EP 2004-12814	A	20040528
US 2004-577043P	P	20040607
WO 2004-EP10161	W	20040910

OTHER SOURCE(S): MARPAT 142:316820
GI



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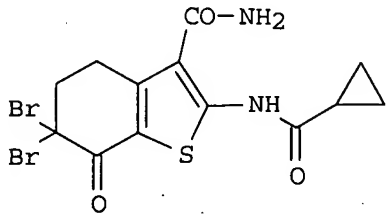


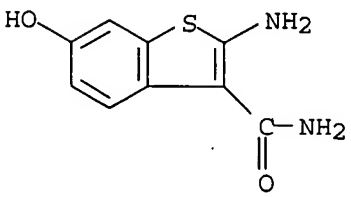
II

AB Described are hetero-bicyclic compds. such as 4,5,6,7-tetrahydro-benzo[b]thiophene-3-carboxylic acid amides, 4,7-dihydro-5H-thieno[2,3-c]thiopyran-3-carboxylic acid amides, 4,7-dihydro-5H-thieno[2,3-c]pyran-3-carboxylic acid amides, or benzo[b]thiophene-3-carboxylic acid amides I, wherein X1 is S, O, NH, substituted nitrogen; Y1-Y4 form with the ring containing X1 a hetero-bicyclic ring system; R1 is H, alkyl, cycloalkyl, heterocycle, alkynyl, substituted Ph, acyl, benzyl; R2 is amide, thioamide, sulfonamide, ester, sulfonyl; R3 is H, acyl, thio-ketone, sulfonyl, amide, thio-amide, diketone-amide, ester, thio-ester; and

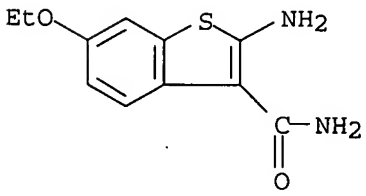
pharmaceutically acceptable salts thereof, the use of these derivs. for the prophylaxis and/or treatment of various diseases such as infectious diseases, including mycobacteria-induced infections and opportunistic diseases, prion diseases, immunol. diseases, autoimmune diseases, bipolar and clin. disorders, cardiovascular diseases, cell proliferative diseases, diabetes, inflammation, transplant rejections, erectile dysfunction, neurodegenerative diseases and stroke, as well as compns. containing at least one hetero-bicyclic compound and/or pharmaceutically acceptable salts thereof. Furthermore, reaction procedures for the synthesis of the hetero-bicyclic compound are disclosed. Thus, benzo[b]thiophen-carboxylic acid amide II was prepared and tested in vitro for its inhibitory effect on mycobacterial protein kinase G (IC50 = 0.1-1.0 μM).

IT 848327-04-8P 848331-75-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of heterobicyclic fused thienopyran compds. as antibacterial antiviral antitumor and pharmaceutically active agents)

RN 848327-04-8 HCAPLUS
CN Benzo[b]thiophene-3-carboxamide, 2-amino-6-hydroxy- (9CI) (CA INDEX NAME)



RN 848331-75-9 HCAPLUS
CN Benzo[b]thiophene-3-carboxamide, 2-amino-6-ethoxy- (9CI) (CA INDEX NAME)



Inventor

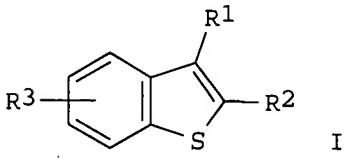
L4 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:991501 HCAPLUS
DOCUMENT NUMBER: 140:27756
TITLE: Preparation of 2-aminobenzothiophene-3-carboxamides as NF-κb inhibitors
INVENTOR(S): Callahan, James F.; Wan, Zehong
PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA
SOURCE: PCT Int. Appl., 34 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

WO 2003104219	A1	20031218	WO 2003-US16876	20030529
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003240935	A1	20031222	AU 2003-240935	20030529
EP 1532135	A1	20050525	EP 2003-731435	20030529
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2005532359	T2	20051027	JP 2004-511289	20030529
US 2006058371	A1	20060316	US 2004-517111	20041203
PRIORITY APPLN. INFO.:			US 2002-386557P	P 20020606
			WO 2003-US16876	W 20030529

OTHER SOURCE(S): MARPAT 140:27756

GI



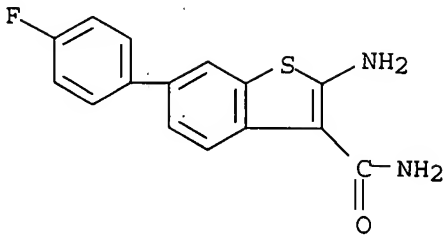
I

AB The title compds. [I; R1 = CONH2; R2 = NR4R5; R3 = H, CN, CF3, halo, etc.; R4 = H, alkyl; R5 = H, CO(alkyl), SO2(alkyl), CONH2, etc.] which are inhibitors of IKK-β phosphorylation of IκB (no data), were prepared E.g., a multi-step synthesis of 2-amino-6-(4-fluorophenyl)benzo[b]thiophene-3-carboxamide (starting from Et 2-amino-4,5,6,7-tetrahydrobenzothiophene-3-carboxylate), was given. The compds. I block pathol. activation of transcription factor NF-κB in which diseases excessive activation of NF-κB is implicated.

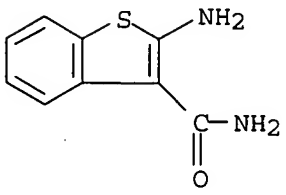
IT 633307-96-7P, 2-Amino-6-(4-fluorophenyl)benzo[b]thiophene-3-carboxylic acid amide
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 2-aminobenzothiophene-3-carboxamides as NF-κb inhibitors)

RN 633307-96-7 HCAPLUS

CN Benzo[b]thiophene-3-carboxamide, 2-amino-6-(4-fluorophenyl)- (9CI) (CA INDEX NAME)



IT 341028-86-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 2-aminobenzothiophene-3-carboxamides as NF-κb inhibitors)
RN 341028-86-2 HCAPLUS
CN Benzo[b]thiophene-3-carboxamide, 2-amino- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> FIL REGISTRY

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	17.81	184.96

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-1.50	-1.50

FILE 'REGISTRY' ENTERED AT 16:11:53 ON 05 NOV 2006

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 3 NOV 2006 HIGHEST RN 912441-38-4
DICTIONARY FILE UPDATES: 3 NOV 2006 HIGHEST RN 912441-38-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

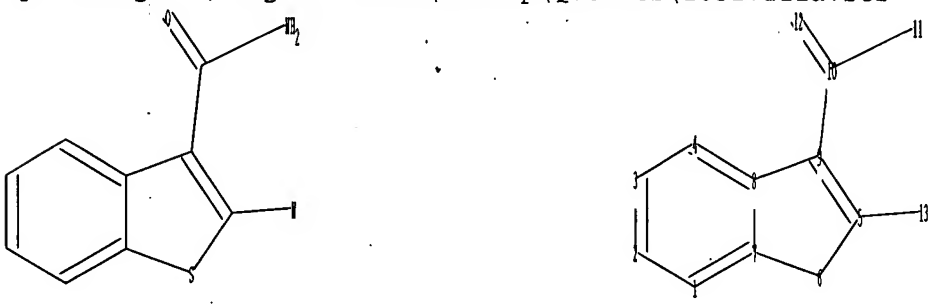
TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10517111a.str

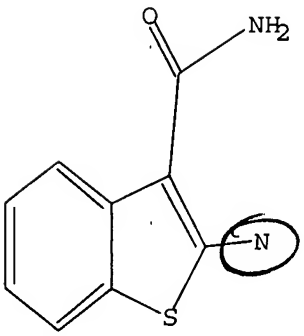


chain nodes :
10 11 12 13
ring nodes :
1 2 3 4 5 6 7 8 9
chain bonds :
5-13 9-10 10-11 10-12
ring bonds :
1-2 1-7 2-3 3-4 4-8 5-6 5-9 6-7 7-8 8-9
exact/norm bonds :
5-13 10-11 10-12
exact bonds :
5-6 5-9 6-7 8-9 9-10
normalized bonds :
1-2 1-7 2-3 3-4 4-8 7-8
isolated ring systems :
containing 1 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS

L5 STRUCTURE UPLOADED

=> d l5
L5 HAS NO ANSWERS
L5 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l5
SAMPLE SEARCH INITIATED 16:12:11 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 36 TO ITERATE

100.0% PROCESSED 36 ITERATIONS 7 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 360 TO 1080
PROJECTED ANSWERS: 7 TO 298

L6 7 SEA SSS SAM L5

=> s l5 sss full
FULL SEARCH INITIATED 16:12:18 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 713 TO ITERATE

100.0% PROCESSED 713 ITERATIONS 132 ANSWERS
SEARCH TIME: 00.00.01

L7 132 SEA SSS FUL L5

=> FIL HCAPLUS
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	166.94	351.90

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-1.50

FILE 'HCAPLUS' ENTERED AT 16:12:42 ON 05 NOV 2006
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FILE COVERS 1907 - 5 Nov 2006 VOL 145 ISS 20
FILE LAST UPDATED: 3 Nov 2006 (20061103/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l7
L8 2 L7

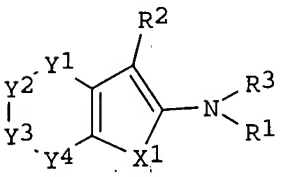
=> d l4 ibib abs tot

L4 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:238994 HCAPLUS
DOCUMENT NUMBER: 142:316820
TITLE: Preparation of hetero-bicyclic fused thieno-pyran compounds as antibacterial, antiviral, antitumor, and pharmaceutically active agents
INVENTOR(S): Koul, Anil; Klebl, Bert; Mueller, Gerhard; Missio, Andrea; Schwab, Wilfried; Hafenbradl, Doris; Neumann, Lars; Sommer, Marc-Nicola; Mueller, Stefan; Hoppe, Edmund; Freisleben, Achim; Backes, Alexander; Hartung, Christian; Felber, Beatrice; Zech, Birgit; Engkvist, Ola; Keri, Gyoergy; Oerfi, Laszlo; Banhegyi, Peter; Greff, Zoltan; Horvath, Zoltan; Varga, Zoltan; Marko, Peter; Pato, Janos; Szabadkai, Istvan; Szekelyhidi, Zsolt; Waczek, Frigyes
PATENT ASSIGNEE(S): Axxima Pharmaceuticals A.-G., Germany
SOURCE: PCT Int. Appl., 259 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005023818	A2	20050317	WO 2004-EP10161	20040910
WO 2005023818	A3	20050825		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2004270394 A1 20050317 AU 2004-270394 20040910
EP 1670804 A2 20060621 EP 2004-786934 20040910
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR
PRIORITY APPLN. INFO.: EP 2003-20616 A 20030910
US 2003-502606P P 20030915
EP 2004-4891 A 20040302
US 2004-551341P P 20040310
EP 2004-12814 A 20040528
US 2004-577043P P 20040607
WO 2004-EP10161 W 20040910
OTHER SOURCE(S): MARPAT 142:316820
GI



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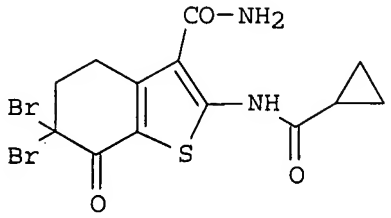


II

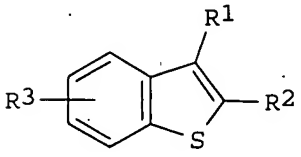
AB Described are hetero-bicyclic compds. such as 4,5,6,7-tetrahydro-benzo[b]thiophene-3-carboxylic acid amides, 4,7-dihydro-5H-thieno[2,3-c]thiopyran-3-carboxylic acid amides, 4,7-dihydro-5H-thieno[2,3-c]pyran-3-carboxylic acid amides, or benzo[b]thiophene-3-carboxylic acid amides I, wherein X1 is S, O, NH, substituted nitrogen; Y1-Y4 form with the ring containing X1 a hetero-bicyclic ring system; R1 is H, alkyl, cycloalkyl, heterocycle, alkynyl, substituted Ph, acyl, benzyl; R2 is amide, thioamide, sulfonamide, ester, sulfonyl; R3 is H, acyl, thio-ketone, sulfonyl, amide, thio-amide, diketone-amide, ester, thio-ester; and pharmaceutically acceptable salts thereof, the use of these derivs. for the prophylaxis and/or treatment of various diseases such as infectious diseases, including mycobacteria-induced infections and opportunistic diseases, prion diseases, immunol. diseases, autoimmune diseases, bipolar and clin. disorders, cardiovascular diseases, cell proliferative diseases, diabetes, inflammation, transplant rejections, erectile dysfunction, neurodegenerative diseases and stroke, as well as compns. containing at least one hetero-bicyclic compound and/or pharmaceutically acceptable salts thereof. Furthermore, reaction procedures for the synthesis of the hetero-bicyclic compound are disclosed. Thus, benzo[b]thiophen-carboxylic acid amide II was prepared and tested in vitro for its inhibitory effect on mycobacterial protein kinase G (IC50 = 0.1-1.0 μM).

L4 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:991501 HCAPLUS
DOCUMENT NUMBER: 140:27756
TITLE: Preparation of 2-aminobenzothiophene-3-carboxamides as NF-kb inhibitors
INVENTOR(S): Callahan, James F.; Wan, Zehong
PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA
SOURCE: PCT Int. Appl., 34 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2003104219	A1	20031218	WO 2003-US16876		20030529
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW					
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
AU 2003240935	A1	20031222	AU 2003-240935		20030529
EP 1532135	A1	20050525	EP 2003-731435		20030529
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK					
JP 2005532359	T2	20051027	JP 2004-511289		20030529
US 2006058371	A1	20060316	US 2004-517111		20041203
PRIORITY APPLN. INFO.:			US 2002-386557P	P	20020606
			WO 2003-US16876	W	20030529

OTHER SOURCE(S): MARPAT 140:27756
GI



I

AB The title compds. [I; R1 = CONH2; R2 = NR4R5; R3 = H, CN, CF3, halo, etc.; R4 = H, alkyl; R5 = H, CO(alkyl), SO2(alkyl), CONH2, etc.] which are inhibitors of IKK-β phosphorylation of IκB (no data), were prepared E.g., a multi-step synthesis of 2-amino-6-(4-fluorophenyl)benzo[b]thiophene-3-carboxamide (starting from Et 2-amino-4,5,6,7-tetrahydrobenzothiophene-3-carboxylate), was given. The compds. I block pathol. activation of transcription factor NF-κB in which diseases excessive activation of NF-κB is implicated.

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> FIL REGISTRY

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	10.54	362.44

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-1.50	-3.00

FILE 'REGISTRY' ENTERED AT 16:13:51 ON 05 NOV 2006

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 3 NOV 2006 HIGHEST RN 912441-38-4
DICTIONARY FILE UPDATES: 3 NOV 2006 HIGHEST RN 912441-38-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

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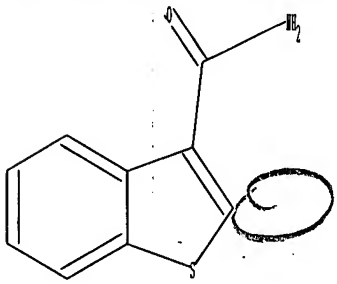

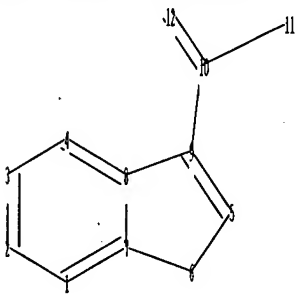

chain nodes :
10 11 12
ring nodes :
1 2 3 4 5 6 7 8 9
chain bonds :
9-10 10-11 10-12
ring bonds :
1-2 1-7 2-3 3-4 4-8 5-6 5-9 6-7 7-8 8-9
exact/norm bonds :
10-11 10-12
exact bonds :
5-6 5-9 6-7 8-9 9-10
normalized bonds :
1-2 1-7 2-3 3-4 4-8 7-8
isolated ring systems :
containing 1 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS 12:CLASS

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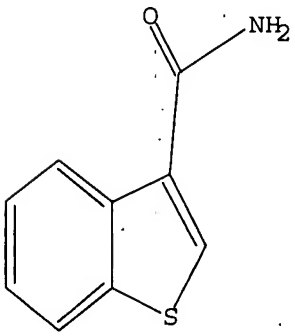

Structure attributes must be viewed using STN Express query preparation.

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SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 2442 TO 3958
PROJECTED ANSWERS: 8 TO 329

L10 8 SEA SSS SAM L9

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100.0% PROCESSED 3037 ITERATIONS 144 ANSWERS
SEARCH TIME: 00.00.01

L11 144 SEA SSS FUL L9

=> FIL HCAPLUS
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	166.94	529.38

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-3.00

FILE 'HCAPLUS' ENTERED AT 16:14:26 ON 05 NOV 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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FILE COVERS 1907 - 5 Nov 2006 VOL 145 ISS 20
FILE LAST UPDATED: 3 Nov 2006 (20061103/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

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L12          15 L11

=> s l12 and py<=2002
      22829455 PY<=2002
L13          11 L12 AND PY<=2002

=> s l13 and nf
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            751 NFS
          46997 NF
                  (NF OR NFS)
L14           0 L13 AND NF

=> d l13 ibib abs hitstr tot
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L13 ANSWER 1 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:719257 HCAPLUS
DOCUMENT NUMBER: 130:3765
TITLE: Intermediates and processes for preparing benzo[b]thiophenes
INVENTOR(S): Misner, Jerry Wayne; Schmid, Christopher Randall
PATENT ASSIGNEE(S): Eli Lilly and Co., USA
SOURCE: PCT Int. Appl., 59 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9848793	A1	19981105	WO 1998-US8510	19980428 <--

W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE,

DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG,
KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX,
NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT,
UA, UG, US, UZ, VN, YU, ZW
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES,
FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI,
CM, GA, GN, ML, MR, NE, SN, TD, TG

CA 2287922	AA	19981105	CA 1998-2287922		19980428 <--
AU 9872614	A1	19981124	AU 1998-72614		19980428 <--
EP 979076	A1	20000216	EP 1998-919936		19980428 <--
R: AT, BE, DE, DK, ES, FR, GB, GR, IT, NL, SE, PT, IE, FI					
JP 2001523253	T2	20011120	JP 1998-547278		19980428 <--
US 6018056	A	20000125	US 1998-69278		19980429 <--
PRIORITY APPLN. INFO.:			US 1997-45131P	P	19970430
			WO 1998-US8510	W	19980428

OTHER SOURCE(S): CASREACT 130:3765; MARPAT 130:3765
GI

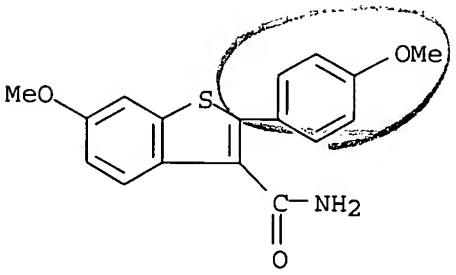
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. [I-III; R = hydroxy protecting group; Y = CO2H, CO2(C1-4 alkyl), C(halo), etc.; A = OH, halo, NO2, etc.; R1 = hydroxy protecting group, H], useful intermediates in the further preparation of pharmaceutical benzo[b]thiophenes, were prepared Thus, reaction of 6-methoxythianaphthen-2-one with p-anisaldehyde in the presence of piperidine in EtOH and THF afforded 45% E/Z-I [R = Me].

IT 215673-40-8P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediates and processes for preparing benzo[b]thiophenes)

RN 215673-40-8 HCAPLUS

CN Benzo[b]thiophene-3-carboxamide, 6-methoxy-2-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 2 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1991:639757 HCAPLUS
DOCUMENT NUMBER: 115:239757
TITLE: Hydantoin derivatives for use as hypoglycemic and/or hypolipidemic agents
INVENTOR(S): Mochida, Ei; Murakami, Kimihiro; Kato, Kazuo; Kato, Katsuaki; Okuda, Jun; Miwa, Ichitomo
PATENT ASSIGNEE(S): Mochida Pharmaceutical Co., Ltd., Japan

SOURCE: Eur. Pat. Appl., 31 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 444546	A1	19910904	EP 1991-102632	19910222 <--
EP 444546	B1	19960911		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
JP 03294270	A2	19911225	JP 1990-43420	19900223 <--
CA 2036902	AA	19910824	CA 1991-2036902	19910222 <--
AU 9171313	A1	19910829	AU 1991-71313	19910222 <--
AU 633694	B2	19930204		
WO 9112803	A1	19910905	WO 1991-JP226	19910222 <--
W: KR				
AT 142493	E	19960915	AT 1991-102632	19910222 <--
US 5202339	A	19930413	US 1991-660562	19910225 <--

PRIORITY APPLN. INFO.:

JP 1990-43420	A	19900223
JP 1987-214549	A	19870828
JP 1989-43422	A	19890225
US 1989-426021	A3	19891024

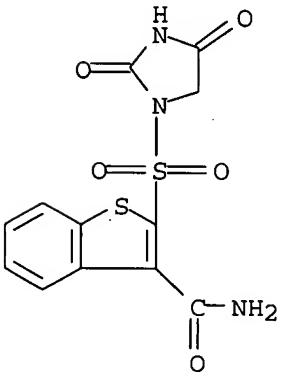
OTHER SOURCE(S): MARPAT 115:239757

AB Pharmaceutical compns. containing hydantoin derivs. are useful for the treatment and prevention of diabetes mellitus with or without hyperlipidemia. Streptozotocin-induced diabetic rats were orally given 1-[benzo(b)furan-2-sulfonyl]hydantoin (I) 100 mg/kg. Serum glucose level 6 h after administration of I was decreased by 52.1 %as compared to 11.0 for gliclazide. Oral formulations and suppositories containing the hydantoin derivs. are given.

IT 128851-53-6
RL: BIOL (Biological study)
(hypoglycemic and hypolipidemic agent)

RN 128851-53-6 HCAPLUS

CN Benzo[b]thiophene-3-carboxamide, 2-[(2,4-dioxo-1-imidazolidinyl)sulfonyl]- (9CI) (CA INDEX NAME)



L13 ANSWER 3 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1991:6501 HCAPLUS
DOCUMENT NUMBER: 114:6501

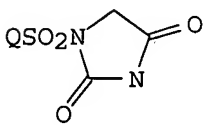
TITLE: Preparation of heterocyclylsulfonylhydantoins as aldose reductase inhibitors
INVENTOR(S): Mochida, Ei; Murakami, Kimihiro; Kato, Kazuo; Kato, Katsuaki; Okuda, Jun; Miwa, Ichitomo
PATENT ASSIGNEE(S): Mochida Pharmaceutical Co., Ltd., Japan
SOURCE: Eur. Pat. Appl., 72 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 355827	A2	19900228	EP 1989-115635	19890824 <--
EP 355827	A3	19900321		
EP 355827	B1	19970102		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
US 4914099	A	19900403	US 1988-235557	19880824 <--
WO 9002126	A1	19900308	WO 1989-JP851	19890822 <--
W: AU, DK, FI, NO				
RW: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE				
AU 8940647	A1	19900323	AU 1989-40647	19890822 <--
AU 623676	B2	19920521		
CA 1338866	A1	19970121	CA 1989-609100	19890823 <--
JP 04128266	A2	19920428	JP 1989-217697	19890824 <--
JP 06015539	B4	19940302		
AT 147073	E	19970115	AT 1989-115635	19890824 <--
ES 2098222	T3	19970501	ES 1989-115635	19890824 <--
US 5004751	A	19910402	US 1989-426021	19891024 <--
NO 9001789	A	19900423	NO 1990-1789	19900423 <--
NO 176478	B	19950102		
NO 176478	C	19950412		
DK 9001001	A	19900614	DK 1990-1001	19900423 <--
US 5232936	A	19930803	US 1991-644632	19910123 <--
US 5202339	A	19930413	US 1991-660562	19910225 <--
AU 9221225	A1	19921015	AU 1992-21225	19920821 <--
AU 646967	B2	19940310		
US 35279	E	19960618	US 1994-197705	19940217 <--

PRIORITY APPLN. INFO.:

US 1988-235557	A	19880824
JP 1989-43422	A	19890225
JP 1987-214549	A	19870828
WO 1989-JP851	A	19890822
US 1989-426021	A3	19891024
JP 1990-43420	A	19900223
US 1991-644632	A5	19910123

OTHER SOURCE(S): CASREACT 114:6501; MARPAT 114:6501
GI



I

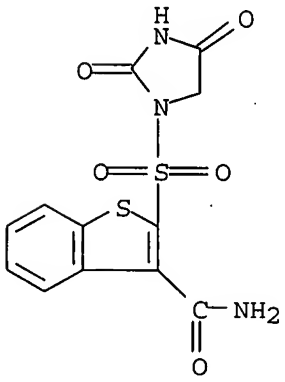
AB Title compds. I (Q = (un)substituted mono- or fused heterocyclyl) salts or solvates were prepared I are useful for treatment and/or prevention of

various forms of diabetic complications based on the accumulation of polyol metabolites. Intermediates for preparing I are also given. Pharmaceutical formulations comprising I are given. To a suspension of ICl in HCl were added 1-(benzo[b]thien-2-ylsulfonyl)-2-thiohydantoin (preparation given) and CH2Cl2 to give I (Q = benzo[b]thien-2-yl). I (Q = 3-bromo-4,6-dichlorobenzo[b]furan-2-yl) also prepared was tested on bovine lens aldose reductase; the IC50 was 0.054 μmol/L vs. sorbinyl whose IC50 was 0.6 μmol/L.

IT 128851-53-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as aldose reductase inhibitor)

RN 128851-53-6 HCAPLUS

CN Benzo[b]thiophene-3-carboxamide, 2-[(2,4-dioxo-1-imidazolidinyl)sulfonyl]- (9CI) (CA INDEX NAME)



L13 ANSWER 4 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1988:150301 HCAPLUS

DOCUMENT NUMBER: 108:150301

TITLE: N-Alkenyl-2-hydroxybenzo[b]thiophene-3-carboxamide derivatives, procedure for their preparation, and their use as dual cyclooxygenase and lipoxygenase inhibitors

INVENTOR(S): Witzel, Bruse E.

PATENT ASSIGNEE(S): Merck and Co., Inc., USA

SOURCE: S. African, 48 pp.
CODEN: SFXXAB

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
ZA 8606993	A	19870429	ZA 1986-6993		19860915 <--
US 4782080	A	19881101	US 1985-776535		19850916 <--
PRIORITY APPLN. INFO.:			US 1985-776535	A	19850916

OTHER SOURCE(S): CASREACT 108:150301

GI For diagram(s), see printed CA Issue.

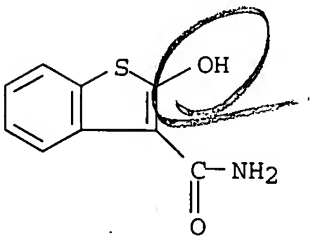
AB Benzothiophenecarboxamides I [R = H, aliphatic group, aryl, (un)substituted Ph, cycloalkyl, haloalkyl, (un)substituted heteroaryl, PhCH2,

phenylalkenyl, or -alkynyl, etc.; n = 0-2; X1, X2, X3, X4 = R; R1, R2, R3 = R, halo; R2R3 = (un)substituted Q [Y = (CH2)n, O, S, SO, SO2, NH]; R4 = R, CR1:CR2R3] or salts, effective cyclooxygenase and 5-lipooxygenase inhibitors and useful as inflammation inhibitors (no data), were prepared by treating II with an N-alkenylation agent R1COCHR2R3, HCOCHR2R3, R0OCH:CR2R3 or R0SCH:CR2R3 (R0 = alkyl, Ph, PhCH2), 2,2-dimethyloxirane, (R0O)2CHCHR2R3, or III (q = 2, 3) in the presence of a strong acid. A mixture of o-mercaptophenylmalonamic acid, DMF, and HCl was heated at .apprx.100° to give II (R = X1 = X2 = X3 = X4 = H) which was heated with Ph2CHCHO, 4-MeC6H4SO3H, and PhMe at 100°, finally at reflux to give I (R = X1 = X2 = X3 = X4 = R1 = R4 = H, R2 = R3 = Ph; n = 0). An ophthalmic formulation comprised 5 mg I and 1 g petrolatum.

IT 113721-54-3, 2-Hydroxybenzo[b]thiophene-3-carboxamide
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with diphenylacetaldehyde)

RN 113721-54-3 HCAPLUS

CN Benzo[b]thiophene-3-carboxamide, 2-hydroxy- (9CI) (CA INDEX NAME)



L13 ANSWER 5 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1976:405441 HCAPLUS

DOCUMENT NUMBER: 85:5441

TITLE: 2-(2-naphthyl)benzo[b]thiophen. Part IV. Further aspects of electrophilic substitution, and ring closures to yield pentacyclic derivatives

AUTHOR(S): Lamberton, Alexander H.; Paine, Richard E.

CORPORATE SOURCE: Dep. Chem., Univ. Sheffield, Sheffield, UK

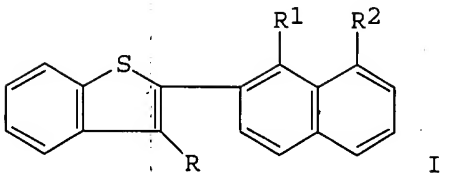
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1976), (6), 683-7
CODEN: JCPRB4; ISSN: 0300-922X

DOCUMENT TYPE: Journal

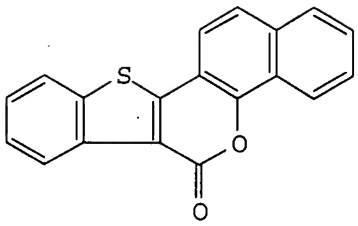
LANGUAGE: English

OTHER SOURCE(S): CASREACT 85:5441

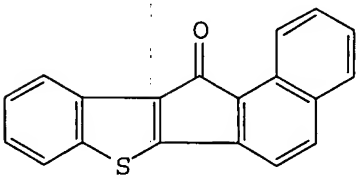
GI



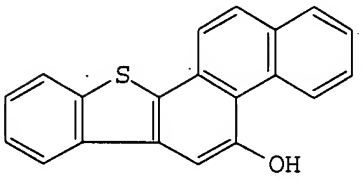
I



II



III



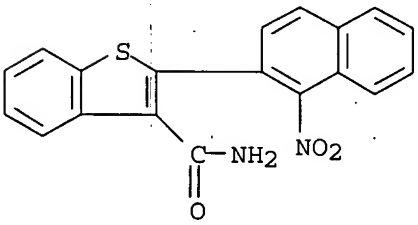
IV

AB The title compound (I; R = R1 = R2 = H), prepared (19-35%) by reaction of benzo[b]thiophene with BuLi and C10H7R (R = 2-F, 1-Cl, 2-Cl), underwent electrophilic attack at the free 3-position on the thiophene ring; however there was no strongly preferred position for further electrophilic substitution. Attempts to decarboxylate I (R = CO2H, R1 = NO2, R2 = H), prepared in 2 steps from the bromobenzothiophene I (R = Br, R1 = NO2, R2 = H), resulted in internal nucleophilic displacement of the NO2 group to give the pentacyclic lactone II. A pentacyclic ketone III and a pentacyclic phenol IV were prepared by Friedel-Crafts ring closures between the benzo[b]thiophene and naphthalene ring system.

IT 59508-03-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

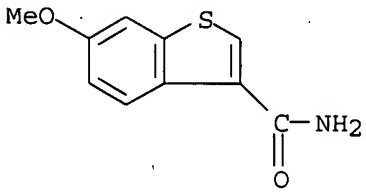
RN 59508-03-1 HCAPLUS

CN Benzo[b]thiophene-3-carboxamide, 2-(1-nitro-2-naphthalenyl)- (9CI) (CA INDEX NAME)

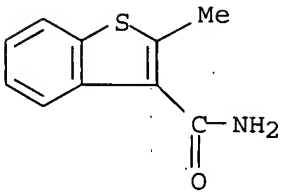


L13 ANSWER 6 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1973:536929 HCAPLUS
DOCUMENT NUMBER: 79:136929
TITLE: 2-Amino-3-(6-methoxybenzo[b]thien-3-yl) propanoic acid
AUTHOR(S): Titus, Richard L.; Titus, Carolyn F.
CORPORATE SOURCE: Dep. Chem., Univ. Nevada, Las Vegas, NV, USA
SOURCE: Journal of Heterocyclic Chemistry (1973), 10(4), 679-81
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English

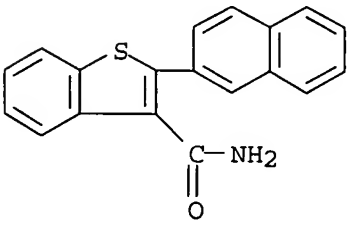
GI For diagram(s), see printed CA Issue.
AB The title compound was prepared by treating 3-MeOC6H4SH with BrCH2COCO2Et, to give 3-MeOC6H4SCH2COCO2Et, which was cyclized to Et 6-methoxybenzothiophene-3-carboxylate. Reduction of the ester to the alc., conversion to the methyl chloride and treatment with MeCONHCH(CN)CO2Et gave the ester I, which was hydrolyzed to the title acid.
IT 43121-89-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 43121-89-7 HCAPLUS
CN Benzo[b]thiophene-3-carboxamide, 6-methoxy- (9CI) (CA INDEX NAME)



L13 ANSWER 7 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1973:71836 HCAPLUS
DOCUMENT NUMBER: 78:71836
TITLE: Formation of pentaatomic lactones on the 2,3-positions of benzo[b]furan, benzo[b]thiophene, and benzo[b]selenophene
AUTHOR(S): Christiaens, L.; Renson, M.
CORPORATE SOURCE: Serv. Chim. Org., Univ. Liege, Liege, Belg.
SOURCE: Bulletin des Societes Chimiques Belges (1972), 81(11-12), 609-22
CODEN: BSCBAG; ISSN: 0037-9646
DOCUMENT TYPE: Journal
LANGUAGE: French
GI For diagram(s), see printed CA Issue.
AB Attempted lactonization of the isomeric hydroxymethyl carboxylic acids I and II (X = O, S, Se) with Ac2O gave only III (X = Se) and IV (X = S, Se). I (X = O, S) and III (X = O) would not cyclize but were acetylated to various degrees. III (X = S) was obtained by cyclizing 2-cyano-3-(hydroxymethyl)benzothiophene. I were prepared by brominating the 3-methyl analogs, subjecting the bromomethyl compds. to Sommelet reaction and NaBH4 reduction II (X = O) was also prepared from the 2-methyl analog, and II (X = S, Se) from their 2-formyl analogs.
IT 39811-93-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(dehydration of)
RN 39811-93-3 HCAPLUS
CN Benzo[b]thiophene-3-carboxamide, 2-methyl- (9CI) (CA INDEX NAME)



L13 ANSWER 8 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1963:59620 HCAPLUS
DOCUMENT NUMBER: 58:59620
ORIGINAL REFERENCE NO.: 58:10151c-d
TITLE: 2-(2-Naphthyl)benzo[b]thiophene. I. Structure, bromination, and nitration
AUTHOR(S): Lamberton, Alex H.; McGrail, P. T.
CORPORATE SOURCE: Univ., Sheffield, UK
SOURCE: Journal of the Chemical Society (1963) 1776-81
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB 2-(2-Naphthyl)-benzo[b]thiophene can readily be isolated as a by-product of the purification of coal-tar naphthalene and is thus potentially available on a tonnage scale. Its structure (I; R = H) has been determined and various derivs., of which the most noteworthy, to date, are I (R = Br, CO2H, NO2, or NH2), have been characterized.
IT 94210-72-7, Benzo[b]thiophene-3-carboxamide, 2-(2-naphthyl)- (preparation of)
RN 94210-72-7 HCAPLUS
CN Benzo[b]thiophene-3-carboxamide, 2-(2-naphthyl)- (7CI) (CA INDEX NAME)



L13 ANSWER 9 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1956:69360 HCAPLUS
DOCUMENT NUMBER: 50:69360
ORIGINAL REFERENCE NO.: 50:12981h-i,12982a-g
TITLE: A new synthesis of thiophenes and condensed thiophenes by ring closure of disulfides
AUTHOR(S): Campaigne, E. E.; Cline, Richard E.
CORPORATE SOURCE: Indiana Univ., Bloomington
SOURCE: Journal of Organic Chemistry (1956), 21, 39-44
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal

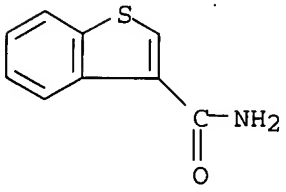
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 50:69360
AB cf. preceding abstract Keeping 2.1 g. 5-phenyl-2-mercapto-2,4-pentadienoic acid (I) and 5 g. iodine in 100 cc. absolute EtOH 14 h. at 20°, diluting the mixture with 2 l. H2O, destroying the excess iodine with NaHSO3, treating the precipitate in 500 cc. 1% NaOH with 4 g. KMnO4 1 h. with occasional stirring, removing the excess KMnO4 with NaHSO3, and acidifying it with HCl give 61% 5-phenyl-2-thenoic acid (II), m. 187-8°; piperidide, prepared via the acid chloride, m. 102-3°; amide m. 197-8°. Refluxing 3 g. II and 12 g. Hg(OAc)2, diluting the mixture with 50 cc. concentrated HCl, steam distilling it, extracting the distillate with Et2O, and subliming the residue of the Et2O extract give 44% 2-phenylthiophene, m. 35-6°. Refluxing 3 g. I 3.5 h. in 50 cc. xylene with 8 g. Cu chromite powder and acidifying the alkaline extract of the xylene solution give 10% II. Keeping 3 g. [SC(CO2H):CHCH:CHPh]2 (III)and 3.8 g. iodine in 75 cc. dioxane 24 h. at 20° gives 68% II. In a similar experiment, when the mixture is refluxed 3 h. and kept overnight, 58% II is obtained. Refluxing 1 g. III and 6 cc. BF3-Et2O 5 h. in 100 cc. dry C6H6, washing the solution with dilute H2SO4, extracting it with dilute NaOH, and acidifying the alkaline solution with HCl give 40% II. The measurement of the rate of consumption of the iodine in the organic solvent shows-that I consumes 1 equivalent of iodine almost immediately while the 2nd equivalent is consumed after 18 h., whereas III requires 18 h. to consume the required 1 equivalent of iodine. The conversion of I to II occurs via III, indicating that, in this case, an acid-catalyzed electrophilic attack of III is involved. The ring closure is promoted by the presence of electron-releasing groups on the aromatic ring. Adding 0.4 g. PhCH:C(SH)CO2H to 4 g. iodine in 30 cc. PhNO2 heated to near-boiling, stirring the mixture vigorously 1 min., cooling and extracting it with NaOH, and acidifying the alkaline solution give 68% benzothiophene-2-carboxylic acid (IV), needles, m. 240-1° (amide, m. 176-7°). In a similar experiment, when 5 g. [SC(CO2H):CHPh]2 and 15 g. iodine in 50 cc. PhNO2 are heated 2 min. at 200°, 61% IV is formed. Refluxing 2.45 g. IV and 8 g. Hg(OAc)2 4 h. in 30 cc. AcOH, adding 10 cc. concentrated HCl, and steam distilling give 16% benzothiophene, leaflets, m. 31-2°. Keeping 2 g. [3,4-MeO(HO)C6H3CH:C(CO2H)S]2 and 2 g. iodine in 75 cc. dioxane 12 h. at 58°, pouring the mixture into 3 l. H2O, decolorizing it with NaHSO3, dissolving the precipitate in dilute NaOH, acidifying the alkaline extract with dilute HCl, extracting with Et2O, and recrystg. the residue of the Et2O extract give 25% 5,6-dimethoxybenzothiophene-2-carboxylic acid (V), plates, m. 260-1° (amide, m. 214-15°). Heating 0.77 g. V and 0.2 g. Cu bronze in 5 cc. quinoline 45 min. at 160-70°, and a few min. at 200° gives 38% 5,6-dimethoxybenzothiophene, m. 99-100°, which gives a deep green color with concentrated H2SO4, a deep violet indophenine test, but no color with Ehrlich reagent. Keeping 2.8 β-2-naphthyl-α-mercaptoacrylic acid and 6 g. iodine in 150 cc. dioxane 24 h. at 50°, pouring the mixture into H2O, and working it up as above give 60% naphtho[1,2-b]thiophene-2-carboxylic acid (VI), needles, m. 257-8°, which is also obtained in 90% yield when 2 g. [2-C10H7CH:C(CO2H)S]2 and 8 g. iodine in dioxane are kept 36 h. at 50°. All attempts at decarboxylation of VI failed to give the

expected thiophene. Keeping 3 g. K3Fe(CN)6 and 0.5 g. 2-C10H7CH:C(SH)CO2H in 50 cc. N NaOH 24 h. at 20°, heating the mixture until the precipitate is dissolved, filtering the hot solution through Norit, and cooling it give 40% Na salt of VI, yellow crystals, from which, on acidification, VI is obtained. Keeping 2 g. α,α'-dithiobis(β-1-naphthylacrylic) acid and 8 g. iodine in 100 cc. dioxane 19 h. at 45° gives 52% naphtho[2,1-b]thiophene-2-carboxylic acid, needles, m. 277-8°, which, on decarboxylation with Cu powder in quinoline at 180°, gives 42% naphtho[2,1-b]-thiophene, plates, m. 113-14°; it gives a dark green indiphenine test with isatin. Possible mechanisms for these acidic and alkaline ring closures are discussed. The UV absorption maximum for the compds. are listed in a table.

IT 858117-17-6, 3-Thianaphthenecarboxamide
(preparation of)

RN 858117-17-6 HCAPLUS

CN Benzo[b]thiophene-3-carboxamide (9CI) (CA INDEX NAME)



L13 ANSWER 10 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1954:11048 HCAPLUS

DOCUMENT NUMBER: 48:11048

ORIGINAL REFERENCE NO.: 48:2038e-f

TITLE: β-Cyanothianaphthene and some of its characteristic reactions

AUTHOR(S): Martynoff, Modeste

SOURCE: Compt. rend. (1953), 236, 385-7

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

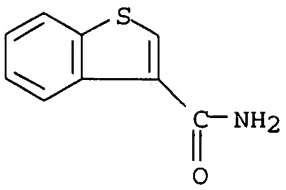
OTHER SOURCE(S): CASREACT 48:11048

AB Heating β-bromothianaphthene and CuCN with pyridine gave β-cyanothianaphthene (I), m. 74°. Warming I with 80% H2SO4 gave 86% of the corresponding carboxamide, m. 198°. Refluxing I with alc. KOH gave 93% of the corresponding carboxylic acid, m. 178°. I with Raney Ni and H then treated with HCl gave 46% di(β-thianaphthenylmethyl)amine-HCl, m. about 220-35°. Condensation of I with MeMgI followed by decomposition with NH4Cl gave β-thianaphthenyl Me ketone, m. 64°; phenylhydrazone m. 97°. Me3CMgCl and I were condensed to give 75% β-thianaphthenyl-tert-butylketimine, b18 186°, m. 68°.

IT 858117-17-6, 3-Thianaphthenecarboxamide
(preparation of)

RN 858117-17-6 HCAPLUS

CN Benzo[b]thiophene-3-carboxamide (9CI) (CA INDEX NAME)



L13 ANSWER 11 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1937:44766 HCAPLUS
DOCUMENT NUMBER: 31:44766
ORIGINAL REFERENCE NO.: 31:6235c-i,6236a-g
TITLE: Phthalocyanines. IX. Derivatives of thiophene, thionaphthene, pyridine and pyrazine, and a note on the nomenclature
AUTHOR(S): Linstead, R. P.; Noble, E. G.; Wright, J. M.
SOURCE: Journal of the Chemical Society (1937) 911-21
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 31:44766
GI For diagram(s), see printed CA Issue.
AB cf. C. A. 31, 1411.7. This series of studies is concerned with the possibility of obtaining similar compds. from heterocyclic instead of aromatic intermediates and efforts to bridge the gap between phthalocyanines and porphyrins. The name phthalocyanine is well established for compds. of the general type indicated by I; it is proposed to use the term porphyrazine for the central ring system of the phthalocyanine mol., i..e., for the structure represented by II; individual compds. are named by attaching a proper prefix; thus the systematic name for phthalocyanine itself is tetrabenzoporphyrazine and the corresponding compound with 4 C5H5N rings in place of 4 C6H6 becomes tetrapyridinoporphyrazine. The formation of porphyrazines from heterocyclic compds. may be expected when (i) they contain the arrangement or are capable of yielding this arrangement easily; (ii) when they possess the necessary thermal stability and no disturbing reactive center in the heterocyclic ring; and (iii) when the heterocyclic system is capable of yielding o-5-membered rings. Thus, porphyrazines should be formed in the following series: thiophene (2,3), thionaphthene, pyridine, pyrazine and probably pyridazine; we should not expect to obtain similar products from the corresponding furan or isooxazole derivs. and the pyrrole, pyrrole and isotriazole systems are doubtful. The preparation of a-methylsuccinic acid in 80-5% yields is described and the preparation from this of 3-methyl- thiophene by fusion of the Na salt with P2S3 in 18-28% yields; slow initial heating appears to be essential; the 2-Ac derivative results in 75-80% yields (contains a little of the 5-Ac isomer). Oxidation of 35 g. of the 2-Ac derivative with alkaline KMnO4 yields 12 g. 3-methylthiophene-2-carboxylic acid, 5 g. thiophene-2,3-dicarboxylic acid (III) and 0.8 g. of the 2,4-dicarboxylic acid; various exptl. conditions and corresponding yields are reported. Attempts to prepare III by direct oxidation of thionaphthene were unsuccessful, the product being recovered unchanged or being completely oxidized. Refluxing III with Ac2O for 30 min. gives the anhydride, m. 140°; the chloride with dry NH3 in C6H6 gives 53% of the diamide, m. 228°, and about 25% of the amic acid (2,3 or 3,2),

m. 238°, yielding with P2O5 the imide, m. 204°. Dehydration of the amide with P2O5 gives 2,3-dicyanothiophene, m. 140°; Ac2O gives the same product but in smaller yield. Heating the dinitrile with CuCl for 10 min. at 230-50° gives a poor yield (due to loss in crystallization from C10H4Cl4) of Cu tetra-2,3-thiophenoporphyrazine, greenish blue powder with faint purple luster; metallic Cu appears to give the same compound, but no pigment was formed with AmONa, litharge or Mg. Attempts to prepare thiophene-3,4-dicarboxylic acid from 3,4-dimethylthiophene and 2,5-dimethylthiophene-3,4-dicarboxylic ester from diacetylsuccinic ester were unsuccessful. Thionaphthenequinone was converted into thionaphthene-2,3-dicarboxylic acid in 75% yields; the acid chloride and NH3 in C6H6 gives about equal quantities of the diamide, m. 204-5°, and of the imide, m. 240°; 2 g. of the amide with Ac2O gives 1.2 g. of 2,3-dicyanothionaphthene (IV), m. 148°; with Ac2O-AcOH there resulted 2(or 3)-cyanothionaphthene-3(or 2)-carboxamide, m. 192-4°; this gives a green pigment when heated with CuCl, Cu or Mg. Heating IV with CuCl at 240-50° for 30 min. gives a tetra-2,3-thionaphthenoporphyrazine, dull green powder, with a faint purple luster; it may contain Cl; the reactions with Al and Mg are also described. Details are given of the preparation of pyridine-2,3-dicarboxylic (quinolinic) acid and of its amide; the latter with Ac2O and AcOH yields 2 (or 3)-cyanopyridine-3(or 2)-carboxamide, m. 255-60°; with Ac2O alone, the yield was lower and there also results the Ac derivative (?) of quinolinimide, m. 150°; 2,3-dicyanopyridine, m. 130°, was prepared by passing the amide through a silica gel catalyst at 320-50° in a stream of dry NH3 gas. Tetra-2,3-pyridinoporphyrazine, blue needles with purple reflex; dimethiodide, greenish blue; Cu derivative, blue; it is soluble in comparatively dilute H2SO4.

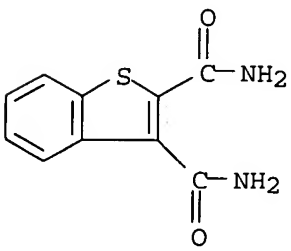
2;3-Dicyanopyrazine (V), m. 132°, was prepared from (H2NCCN)2 and (CHO)2; the 5,6-di-Me derivative, light yellow, m. 166°, was prepared from Ac2; benzil gives the 5,6-di-Ph derivative, m. 245°; phenanthraquinone yields 2,3-dicyanophenan- thra(9',10',5,6)pyrazine, golden, m. 320°. V and CuCl give Cu tetrapyrazinoporphyrazine tetrahydrate((precipitated from H2SO4 by ice), blue with purple luster; drying over H2SO4 gives the trihydrate; 2 H2O were lost at 150° and 3 at 200°; the monohydrate forms the trihydrate in the air; the Mg compound, blue on solution in concentrated H2SO4 and precipitation with H2O, yields the free

Porphyrazine, as the tetrahydrate, a blue powder. The derivs. of V yield colored solids with AlCl3, Cu, CuCl and ZnCl2, which were not examined in detail.

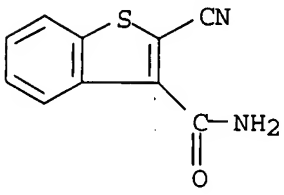
IT 857547-91-2, 2,3-Thianaphthenedicarboxamide 857548-04-0, 3-Thianaphthenecarboxamide, 2-cyano-
(preparation of)

RN 857547-91-2 HCAPLUS

CN 2,3-Thianaphthenedicarboxamide (4CI) (CA INDEX NAME)



RN 857548-04-0 HCAPLUS
CN 3-Thianaphthenecarboxamide, 2-cyano- (4CI) (CA INDEX NAME)



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FULL ESTIMATED COST	61.27	590.65

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
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